

# Review of: "A Novel One-Pot Three-Component Approach to Orthoaminocarbonitrile Tetrahydronaphthalenes Using Triethylamine (Et<sub>3</sub>N) as a Highly Efficient and Homogeneous Catalyst Under Mild Conditions and Investigating Its Anti-cancer Properties Through Molecular Docking Studies and Calculations"

Clarina N'Da<sup>1</sup>

<sup>1</sup> North-West University

Potential competing interests: No potential competing interests to declare.

**Review manuscript entitled: "A Novel One-Pot Three-Component Approach to Orthoaminocarbonitrile Tetrahydronaphthalenes Using Triethylamine (Et<sub>3</sub>N) as a Highly Efficient and Homogeneous Catalyst Under Mild Conditions and Investigating Its Anti-cancer Properties Through Molecular Docking Studies and Calculations".**

Some improvements have been made from the first draft with regard to the chemistry and tables, but it still needs editing.

The chemistry is better presented but should be separated from the molecular docking studies, which, in my opinion, still need to be investigated with other appropriate proteins.

The ADME data in Figure 4 incorporated into the docking calculations should be separated, as docking studies highlight the interaction of compounds at the molecular level with the protein or enzyme targeted.

Authors must disclose the molecular modelling software used and the preparation method so interactions can be visualized by others. The supplementary information showing <sup>1</sup>H spectral data along with the interaction between the ligand (the compound) and the protein is insufficient.

Biological evaluation as an anticancer agent by in vitro assays using known cell lines, including toxicity studies of these compounds, should be determined.

A discussion section must be done that fully describes the molecular modelling studies and biological evaluation of compounds as ant-cancer agents. Theoretical calculations are good but not sufficient to draw conclusions involving biological systems.

This manuscript is still a work in progress.

The authors must take the comments of reviewers into serious consideration so all can benefit from such research.

Thanks,

